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RPPR Final Report
as of 02-Oct-2017

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STEM Degrees: **STEM Participants:**

Major Goals: ARO Workshop
Characterizing the Dynamics of Geo-Surface Materials: Modeling and Simulation Challenges and Opportunities

Goal. This workshop's goal is to : (a) identify open problems that pertain to the dynamics of geo-surface materials; and (b) understand whether recent fundamental advances in geophysics, applied mathematics, and computational science can combine in a multi-disciplinary fashion to produce a breakthrough in the broad area of geo-surface dynamics characterization. The outcome of this workshop will be a technical report identifying a set of multi-disciplinary basic research thrusts that can lead to breakthroughs in our understanding of issues related to the topic of interest.

Rationale. Recent theoretical, algorithmic, and advanced computing breakthroughs are providing a fresh opportunity to revisit several open problems pertaining to the modeling and simulation of the dynamics of geo-surface materials. Assuming a broad range of forms - from dry/saturated sand to silt to clay - the problem of interest brings to the fore unique modeling and simulation challenges at the interface of applied math (homogenization, handling of discontinuous behavior, discrete vs. continuum representations, fluid-solid interaction, plasticity aspects), computer science (large scale simulation, parallel computing), and practical application (soft-matter physics, machine-ground interaction).

Anticipated Topics of Discussion. The discussion will include but not be limited to the following set of topics:
a) Visco-elasto-plastic continuum models of geo-surface materials
b) Discrete models of geo-surface materials (rocks/gravel/sand)
c) Mixed continuum-discrete representations. Coarse-graining and fine-graining mathematical formulations
d) Multi-physics aspects related to the modeling of saturated soils (fluid-solid interaction issues)
e) Modeling and simulation of frozen/thawing/snow-covered soils
f) Mathematical methods and algorithmic efficiency for large-scale problems
g) High performance computing aspects: handling temporal and spatial multiple scales
h) Legacy software development challenges posed by emerging computational architectures
i) Uncertainty quantification
j) Big data issues related to geo-surface materials characterization and visualization
k) Machine-ground interaction and terramechanics aspects
l) Broader impact and synergistic aspects tying the proposed topic to open practical problems
m) Model validation aspects

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Objectives. Bring together scientists from academia, government labs and industry in order to
1. Get a better understanding of the state of the art in geo-surface materials modeling and simulation
2. Identify relevant gaps in (i) modeling techniques, (ii) numerical solution methods, and (iii) advanced computing software & hardware support
3. Produce a set of recommendations subsequently summarized in a technical report that states the open problems, identifies possible solutions, and suggests a future course of action

Aspects Related to Broader Impact. Although the workshop will concentrate primarily on the topic of geo-surface materials characterization, modeling and simulation advances made in this area are expected to impact a wide range of areas such as granular flows, additive manufacturing, composite materials, pyroclastic flows, formation of asteroids and planets, meteorite cratering; and also industries such as farming, food processing, pharmaceuticals, chemical and biological engineering, manufacturing, off-road mobility, construction and mining.

Logistics. Dates: August 17-18, 2016. Schedule: Day 1 – start meeting at noon, run through 6 PM. Day 2 – commence at 8 AM, wrap up at 5 PM. Organizers: Dan Negrut of University of Wisconsin-Madison and Ken Kamrin of MIT. Venue: Courtyard Marriot Downtown Chicago/River North (30 East Hubbard Street, Chicago, IL 60611 USA). Anticipated attendance: 15-25 scientists.

Accomplishments: The meeting was organized for two days in Chicago.
The participants involved in this event were as follows:
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Training Opportunities: Nothing to Report

Results Dissemination: A website was set up to share with the community at large all the presentation made at the workshop.
Workshop website: http://outreach.sbel.wisc.edu/Workshops/GPUworkshop/2016-ARO/

Honors and Awards: Nothing to Report

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URL: http://outreach.sbel.wisc.edu/Workshops/GPUworkshop/2016-ARO/
Date Received: 29-Sep-2017
Title: ARO Workshop, Chicago, IL
Description: 2016 Chicago ARO Workshop Characterizing the Dynamics of Geo-Surface Materials: Modeling and Simulation Challenges and Opportunities

Summary of Workshop Outcomes

Characterizing the Dynamics of Geo-Surface Materials: Modeling and Simulation Challenges and Opportunities

August 17-18, 2016

We have identified obstacles and opportunities for breakthroughs in four areas listed below.

AREA 1: DATA COLLECTION

Where we are now – **data collection**

Up until very recently, data collection has been done by one of the following three alternatives:

(i) Rely on particle image velocimetry (PIV) in 2D flows. However, this is most often not sufficient for what we need – the real world is not 2D. Moreover, one would have to change the nature of the system to be able to put a plastic wall where you need to notice what happens, a step that interferes with the dynamics of the system.

(ii) One could look at boundary behavior of 3D flows (how the surface flows, deforms, etc.).

(iii) One can run DEM tests and consider these simulation results as "ground truth". The problem is that by and large, the penalty methods that are almost exclusively used in DEM rely on a Herz type theory that only applies for a narrow spectrum of scenarios.

Perceived obstacles – **data collection**

It has proven very difficult to get position/velocity/stress information in a 3D mixture of granular material; i.e., from *inside* a granular material. Recall that granular material spans multiple spatial scales – from powders to avalanche dynamics to formation of asteroids, and getting "inside" is very difficult as application fields work on quite different scales. Without experimental data to guide the scientific progress we are limited to writing papers advancing theories that we can't validate. What we are seeking are techniques that provide information in a time-varying 3D context without disturbing too much the dynamics of the system being measured. It is increasingly more difficult to obtain (in this order) position information, velocity information, and frictional/contact force information. All these quantities are needed for moving away from phenomenological models and establishing a quantitative approach to characterizing the dynamics of interest.

Opportunities to make progress – **data collection**

We have two new and promising ways to collect experimental data. Miniaturization, an immediate benefit of Moore's Law, has recently led to sensors that are so small that they can be inserted in a system of interest to collect data with minimal distortion of the underlying system dynamics (UC Berkeley/Cambridge). Likewise, X-ray computed tomography, where we can track motion and loading at the grain level, allows us for the first time to collect data at this level of resolution (Grenoble, France). These experimental capabilities are robust enough to let us go inside particle processes as they happen and record the field observables that are needed to produce quantifiable models. We anticipate that these models, for real 3D materials, will open up an unprecedented opportunity to quickly and accurately predict large-scale processes (e.g. geological and terramechanical flows) that move beyond empirical/phenomenological interpretations of the phenomena of interest. As a side note, these novel experimental techniques were developed outside US. The sensor-based approach has been developed at Cambridge (the faculty, who participated in the workshop, moved as of this year to UC Berkeley), while the X-ray computed tomography technique was developed in France. Workshop participants from CalTech and Columbia are collaborating with the French scientists to obtain data from them.

AREA 2: MODELING AND NUMERICAL APPROACHES

Where we are now - **modeling and numerical approaches**

DEM is almost exclusively the tool of the trade in characterizing the dynamics of geo-surface materials. The DEM force model draws on a Herz/Mindlin theory applicable for sphere-to-plane and sphere-to-sphere scenarios. Several recent theories extend these "discrete approach" scenarios to more complex primitives (cylinders and ellipsoids) but yet far from the broad spectrum of shapes that nature confronts us. Beyond the discrete approach, several attempts have been made to using continuum methods to capture the dynamics of geo-surface materials. A class of approaches attempts to use a non-local rheology to formulate a continuum problem. Another class of approaches uses a finite element approach which is informed by DEM simulations run at some key locations on an "as-needed" basis. Somewhere in between the two approaches; i.e., discrete at one end of the spectrum and continuum at the opposite end, there have recently been approaches that suggest a mixing of the two approaches via arelquin coupling. In this context, one would have a discrete representation in some regions, which is interfaced via appropriate boundary conditions to a continuum representation in complementary regions.

Perceived obstacles - **modeling and numerical approaches**

A. The homogenization approach has proved a frustrating exercise, which led to Nature papers with theories that touted the solution of the problem at hand. However, most of these theories ignored the nonlocal nature of the frictional contact problem, which turned out to play a very important role in the physics at hand. This has not been recognized until two or three years ago. It looks obvious today, but for the longest time we couldn't produce good results since in coming up material laws (constitutive equations) we were looking at what happened at one point. We need to look in a neighborhood and this is raising additional challenges.

B. Penalty methods in DEM are limiting in the class of scenarios that we can simulate: simple geometries for which the two body frictional contact theory has a clearly defined solution (of the Herz type, for instance). The obstacle here is to identify new modeling techniques that allow us to treat the frictional contact problem in such a way that allows us large integration time-steps and handling of arbitrary geometries (not only sphere-to-sphere, sphere-to-plane, etc.). The frictional contact problem needs to be formulated differently, and new classes of numerical methods should be invented to effectively handle the new set of dynamics equations to allow accurate simulation at large time steps (DEM is limiting us at step-sizes of the order 1E-6 to 1E-4; this poses an obstacle insofar the length of the simulations we can run at steps sizes that are this small).

C. Regarding idea of dimensionless analysis to enable the emulation of macro-scale phenomena via micro-scale experiments: this is something that we simply don't know how to do because no effort has gone into it. A prerequisite for any investigation in this area is a wealth of experimental data, which we are now about to get access to, see 1) above.

D. There is no clear understanding of several "young" methods such as SPH and MPM. Our understanding has holes since not much effort has gone into the convergence, efficiency, and scalability analysis of these methods. New basic applied math tools need to be established and used to figure out how to impose compatible boundary conditions, how to better approximate the gradient and Laplacian information in these meshless methods, whether multi-grid solvers are applicable, what sort of splitting techniques (a la Chorin) work, etc.

E. Lack of data, sheer amount of data processing that goes into this task, lack of sufficiently developed machine learning techniques, the multi-disciplinary attribute of the undertaking

<u>Opportunities to make progress - **modeling and numerical approaches**</u>

A. For the first time we have in nascent form a promising theory for representing the collective dynamics of large systems of discrete elements using a continuum approach. This homogenization approach has been recently developed at MIT by a workshop participant. It's by no means complete (discrete elements should be more or less monodisperse spheres, the regime needs to be steady state, saturation is not accounted for) but it is a very good beginning that is rooted in a solid scientific method: experimental data and/or fully resolved, small scale, simulations are used to produce material models for continuum representations of discrete flows.

B. A new approach to handling contact and friction that is variational in nature and falls back on complementarity constraints looks very promising when compared to the almost universally embraced penalty approach in use today. The differential variational inequality approach allows for large integration time-steps in the Discrete Element Method (DEM) since it doesn't introduce high stiffness in the problem; second, it provides a versatile framework to better capture plasticity and non-penetration conditions. Finally, we are starting to recognize that this complementarity-based approach is more broadly applicable and that from a numerical solution standpoint it can be successfully tackled with new methods that are coming out in the nonlinear numerical optimization community.

C. One emergent theme within the community promotes the idea of dimensionless analysis to enable the emulation of macro-scale phenomena via micro-scale experiments. This is in the vein of using Reynolds numbers in CFD, an idea that allowed to understand how airplanes behave by measuring in a wind-tunnel and/or simulating small-scale replicas that are 1/1000 the size of the original system. The interesting connection here would be to look at small granular systems to understand how tectonic plates move or how earthquake wave propagate through the earth's mantle

D. There are new ways of characterizing the fluid-solid interaction that draw on non-traditional approaches. Specifically, there is great interest in Lagrangian methods for capturing the dynamics of the continuum phase. These methods are not clearly understood but offer a manifestly different take on physics that are not easily captured with traditional Lagrangian mesh-based or Eulerian approaches. The families of methods that were most often cited as being complementary to the establish techniques are the Material Point Method (MPM) and Smoothed Particle Hydrodynamics (SPH). The former is an ALE method that doesn't have the valence problems associated with the latter. Both are attractive owing to their ability to capture free surfaces, both fluids and deformable solids, and are akin to the DEM methods that are widely used in our community.

E. There is renewed interest in reduced order models that is unrelated to the discrete-to-continuum thrust mentioned at (a) above. One theme that emerged at the workshop was that no matter how fast the computers are, DEM simulation in terramechanics is presented with a similar set of challenges that turbulence poses to the Navier-Stokes equations. We can do Direct Numerical Simulation (DNS) of Navier-Stokes at a research level, but not for practical engineering problems — and we'll probably never be able to. What DEM *can* provide us with at a level never before possible is access to detail and quantities that we can't get from experiments alone, and this in turn can guide the development of reduced-order models that can be deployed to solve challenging real-life applications.

AREA 3: EMERGING HARDWARE ARCHITECTURES

<u>Where we are now - **hardware**</u>

We have recently passed or are about to witness three remarkable milestones.

(i) In about five years (2021) Moore's Law will cease to apply by virtue of the feature length reaching the 5 nm limit beyond which the laws of physics suggest that our current computing model will stop working.

(ii) For the first time we have been in a position to use 3D stacked memory which ushers in extremely high bandwidth speeds and very low latency at a fraction of the real-estate required by today's DRAM designs. Indeed, while between 1984 and 2015 the memory speed has increased year-to-year at a pace of approximately 1.07; i.e., 7%, during the last 12 months we witnessed a significant jump that saw bandwidths increase by a factor of 4. Moreover, the amount of power required by memory went down significantly, the amount of space occupied is manifestly smaller (about 16 times smaller, owing to stacking in the z direction), and the latency is smaller due to the way in which the memory is controlled and also to the shorter distances needed to move data when using through silicon vias (TSVs).

(iii) A fast GPU accelerator (mostly out of NVIDIA) or CPU accelerator (Intel Xeonn Phi) possesses flop rates that are on par with those of the fastest supercomputers in the world a decade ago. These accelerators also tout global memory bandwidths and latencies which are one to two orders of magnitude better when compared to the system memory of a traditional laptop/workstation.

Perceived obstacles - **hardware**

Lack of adequate hardware that allows the conclusion in reasonable amounts of time of our memory-bound simulations, which are characterized by large amounts of data movement. DEM is not compute bound; collision detection, book-keeping, and shuffling data around in memory is what takes most of the time (at least as far as the current numerical solutions and their implementations are concerned)

Opportunities to make progress - **hardware**

The size of the problems solved in this field are typically daunting. If possible, we would like to attack problems with billions of degrees of: particle-laden flows, partially saturated soils in various regimes (pendular, capillary, funicular, suspension), large granular problems, soil freezing/melting, etc. We are on the brink of experiencing a significant increase in memory speed that we posit to have a significant impact in our field. The fact that the system memory speed will increase by a factor of four to five times bodes well for our push to ever-larger simulations. Note that this issue is relevant not only in geo-simulation, but also in experimental-data processing where for instance an X-ray measurement experiment in granular material produces vast data sets that have to be post-processed in a machine learning framework for feature extraction. The fact that we have access to parallel computing via accelerators (GPU, Intel Xeon Phi) and to high bandwidth memory (HBM) via recently introduced 3D chip designs is poised to catalyze the computationally-hungry DEM approach

AREA 4: SOFTWARE SOLUTIONS

Where we are now - **software**

We have an open source software called LAMMPS (Sandia National Lab), which is used for molecular dynamics but retrofitted to handle granular dynamics should the discrete elements be all spheres of roughly similar sizes. There are also several commercial codes called EDEM (Scotland) and ITASCA (USA). They are both relatively slow and have limited support for parallel computing, which adversely impacts their scalability. Finally, there is a software tool called LIGGGHTS (Austria), which is partially open source (open source for small systems) and is built on top of LAMMPS. All these packages are focused exclusively on the dynamics of discrete elements, most often using a penalty approach. The weak point of all these codes is that they can’t address the multi-physics dimension at play in the dynamics of geo-surface materials. For instance, fluid-solid interaction aspects, continuum models for plasticity to augment the discrete representation, dual formulation (discrete-continuum), support for other implements such as robots, vehicles, etc. Recently, the BSD3 open source code Chrono has emerged as a contender in that it has support for granular dynamics, continuum representations (nonlinear finite element analysis support for beams, shells, volumetric elements, w/ support for plasticity), and traditional mechatronics applications.

Perceived obstacles - **software**

It takes a village to produce a meaningful piece of code that can be used by a community to advance our collective understanding of the field. For instance, a software framework has to deal with: code development; Source management + Build management + Unit Test management; handling pull requests (if larger project w/ collaborators); hardware landscape in flux (CUDA/OpenCL/OpenACC/OpenMP/MPI/Charm++); documentation; prepare and execute releases across multiple platforms (Windows, Mac OsX, Linux); Bug fixes/Profiling/Code optimization; user forum (hand-holding, extremely time consuming); establish/maintain/expand library of models for user adoption; user conferences. The importance of having access to adequate simulation tools is on par with that one of having access to sharper experimental techniques to collect data.

Opportunities to make progress - **software**

The software infrastructure that supports the broad field of geo-surface materials dynamics has matured significantly over the last decade. We can carry out reasonably fast million body simulations that are feature-rich. That is, we don't have only a bunch of granular material and nothing else in the simulation. Instead, the systems analyzed are multifaceted: vehicle moving through mud, beach erosion, biomimetic robots moving over granular terrain, shock propagation in poly-disperse and heterogeneous materials, etc. We are increasingly having access to a repository of open source simulation packages that enable the analysis of real-life problems to the point where we can produce data that is impossible or extremely challenging to obtain through physical testing.

SUMMARY OF POTENTIAL PAYOFFS

The interplay between *new experimental data collection techniques*, *emerging classes of numerical methods*, *increasingly versatile open source simulation packages*, and *imminent leaps in computer/memory architecture* is poised to lead in the immediate future to breakthroughs relevant over an incredibly broad range of scales, both in science and engineering. For instance, at macroscale, we would be in a position to investigate:

- How landscapes are made of geomaterials and shaped by flows of geomaterials
- Rate laws for erosion and sediment transport depend on constitutive properties of granular materials: creeping soils, landslides, debris flows, bedload and suspended load sediment transport in rivers. Models of these processes will benefit from improved understanding of granular phenomena.
- Several of the processes above are also natural hazards, e.g., avalanches, shore collapse, beach erosion, pyroclastic flows, etc.
- Explicit, mechanistic models of granular phenomena could allow us to predict surface properties in planetary environments, where empirical calibrations based on Earth materials commonly fail.
- Characterizing the rheology of natural materials is one of the biggest challenges in the study of Earth's surface, and even extends to the breakdown of rock that generates granular materials. This highlights one way in which the study of granular mechanics stands to benefit from geoscience: a better understanding of the controls on grain size, shape and composition of natural materials will help parameterize granular models in general, as well as models designed to be applied to specific sites.

At the opposite end of the spectrum, at microscale/mesoscale, we'll be better positioned to investigate:

- Self-assembly: Due to scaling of fabrication processes, self-assembly is a necessity for fabricating large quantities of designer, micro- and nanostructured materials. Such processes typically involve billions of particles. Currently the complexity that is achievable by self-assembly is highly limited.
- Energetic materials: Many energetic materials (explosives, solid rocket propellant) are micro- to nanoscale granular materials. Energetic material response is dictated by highly nonlinear stress wave propagation (including localization and delocalization).
- Shock/impact/vibration mitigation via granular inspired designer materials: typically involve dynamic (and often nonlinear) processes, e.g. spall.
- Understanding geological material blast response. This is a highly nonlinear process.
- Acousto- optic/plasmonic functional materials: when the particle length scale approaches or is below that of light, acoustic and electromagnetic wave interaction is enhanced. Applications could include ultrafast optical modulators, or optically responsive materials (camouflage).
- Designer phononic (thermal materials): there are direct analogies between thermal phonon transport through atomic lattices/glasses and vibrations in granular materials. When the length scale of granular media is reduced to approach the near-atomic scale, there may be the opportunity for creating designer materials with tailored thermal properties

Stepping aside from the ends of the spectrum, there are multiple applications “in the middle” of the scale where we can open up new avenues for investigation. Indeed, more than 50% of the material manipulated in industry comes in bulk form. Other applications and areas of research that stand to benefit from advances in the field of interest are

- Ground vehicle mobility over a variety of terrains
- Better understanding of biomimetic robots operating in rough terrain
- Vehicles at very high speeds: Understanding dynamic friction processes (e.g. Shallamach waves) in the setting of complex granular media
- Applications in food industry
- Additive manufacturing and 3D printing